

Tamm's surface states and Bose-Einstein condensation

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We calculate and discuss the effects on the thermodynamic properties of a 3D Bose gas caused by a gap Δ in the energy of the particles constituting the gas that without the gap behaves like an ideal Bose gas. Explicit formulae with arbitrary Δ values are discussed for: the critical temperature which increases as the gap grows; the condensate fraction; the internal energy; and the constant-volume specific heat found to possess a jump-discontinuity for any Δ different from zero. Three dimensional infinite ideal Bose gas results are recovered when the energy gap goes to zero.

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I. INTRODUCTION

After the discovery of helium superfluidity by Kapitza and Allen independently [1, 2], London [3] proposed that this novel phenomenon could be a consequence of the Bose-Einstein condensation (BEC) predicted by Einstein in 1925 [4]. London himself calculated the critical temperature of a 3D ideal Bose gas with mass and density equal to that of helium four; the critical temperature obtained is 3.2 K, which is very close to the temperature at which helium four becomes superfluid, i.e., 2.17 K. This result feed the idea that helium superfluidity was motivated by a BEC of the helium atoms. However, the specific heat of helium four near absolute zero temperature had been observed and measured [5] to increase exponentially with temperature which is not expected for a 3D ideal Bose gas whose specific heat increases proportional to $T^{3/2}$. To reproduce this exponential behavior with temperature, an artificial gap in the dispersion relation was introduced [6, 7]. Although the exponential behavior is reproduced for low temperatures, the critical temperature increases beyond the Bose-Einstein critical temperature when the energy gap increases. This behavior is contrary to what is observed in helium, where the interaction reduces the superfluidity critical temperature below the 3D BEC critical temperature when the density is that of liquid helium four. Although many theoretical efforts [8] have been made to justify the gap as a result of interactions among the particles, the gap not only has not showed up but there are arguments against its existence [9].

Now days, when it is possible to reproduce almost any space lattice structure trapping fermions or bosons in the laboratory, we consider relevant to reconsider the surface effect on the dispersion relation of quantum particles placed in optical periodic lattices which simulate crystalline solids. Many year ago, after the publication of the Kronig-Penney model [10] for an infinite solid, Tamm [11] discussed the finite size effect on the particle energy spectrum using a semi-infinite idealized one-dimensional crystal. Tamm reported the occurrence of an isolated energy level for each allowed energy band. These isolated

surface level are called Tamm's surface states.

In this article we return to the London's idea to introduce a gap in the energy spectrum of bosons but keeping in mind the existence of Tamm surface states, to give details of the energy gap effects on the Bose-Einstein critical temperature, its isochoric specific heat as a function of temperature as well as the its specific heat jump at T_c .

In Sec. II after definition of the system, we calculate: a) the critical temperature as a function of gap; b) condensed fraction. In Sec. III we give the following thermodynamic properties: the internal energy, the isochoric specific heat as a function of temperature and the jump height of the specific heat at T_c . In Sec. IV we give our conclusions.

II. BOSE GAS WITH DISPERSION RELATION PLUS A GAP

Our system is a 3D infinite Bose gas of N particles of mass m whose energy as a function of its momentum $\hbar k$, i.e. its dispersion relation, is given by

$$\varepsilon_k = \begin{cases} \varepsilon_0 & \text{if } k = 0 \\ \varepsilon_0 + \Delta + \hbar^2 k^2 / 2m & \text{if } k > 0 \end{cases}, \quad (1)$$

For a finite temperature the particle number N is distributed between the energy ground state and the excited states, i.e., $N = N_0(T) + N_e(T)$ with

$$N_0(T) = \frac{1}{e^{\beta[\varepsilon_0 - \mu(T)]} - 1},$$

the particles in the energy ground state and

$$N_e = \sum_{\mathbf{k} \neq 0} n_k = \sum_{\mathbf{k} \neq 0} \frac{1}{e^{\beta[\varepsilon_k - \mu(T)]} - 1}, \quad (2)$$

the particles in the excited states, with $\beta \equiv 1/k_B T$, and $\mu(T) \leq \varepsilon_0$ the chemical potential.

In the thermodynamic limit sums in (2) are well approximated by integrals and after defining $\xi \equiv \beta \hbar^2 k^2 / 2m$

then $d\xi = (\beta\hbar^2/2m)2k dk$ and $\xi^{1/2} = (\beta\hbar^2/2m)^{1/2} k$, Eq. (2) becomes

$$\begin{aligned} N_e &= \frac{L^3(2m/\hbar^2)^{3/2}}{4\pi^2\beta^{3/2}} \int_0^\infty \frac{\xi^{1/2}d\xi}{e^{-\beta(\mu-\varepsilon_0-\Delta)} e^\xi - 1} \\ &= \frac{L^3(2m/\hbar^2)^{3/2}}{4\pi^2\beta^{3/2}} g_{3/2}(z_1)\Gamma(3/2) \end{aligned} \quad (3)$$

with $z_1 \equiv \exp[\beta(\mu - \varepsilon_0 - \Delta)] \leq 1$.

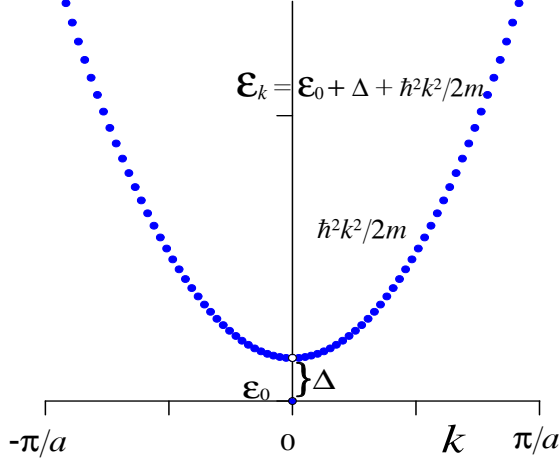


FIG. 1: Particle energy.

A. CBE critical temperature

The critical temperature T_c is the smaller temperature for which $N_e(T_c) = N$ and as a consequence $\mu(T_c) = \varepsilon_0$, therefore

$$N = \frac{L^3(2m/\hbar^2)^{3/2}}{4\pi^2\beta_c^{3/2}} g_{3/2}(z_{1c})\Gamma(3/2) \quad (4)$$

with $z_{1c} \equiv \exp[-\beta_c\Delta] \leq 1$. For $\Delta = 0$, $z_{1c} = 1$ and we recover the critical temperature T_0 of a ideal Bose gas via the relation

$$N = \frac{L^3(2m/\hbar^2)^{3/2}}{4\pi^2\beta_0^{3/2}} \zeta(3/2)\Gamma(3/2) \quad (5)$$

with $\beta_0 = 1/k_B T_0$ and T_0 the BEC critical temperature for a ideal Bose gas with a number density equal to that of our system. Note that in this case the dispersion relation for the Bose gas starts at ε_0 but has no effect on the critical temperature as this is a translation of the starting point of the particle energies.

For $\Delta \neq 0$, from the ratio between (4) and (5),

$$\begin{aligned} 1 &= \frac{\beta_0^{3/2} g_{3/2}(z_{1c})}{\beta_c^{3/2} \zeta(3/2)} \\ \text{or} \quad T_c &= \left(\frac{\zeta(3/2)}{g_{3/2}(z_{1c})} \right)^{2/3} T_0 \end{aligned}$$

Considering that $\zeta(3/2)/g_{3/2}(z) \simeq 1 + (3/2)(1-z)^{1/2} +$

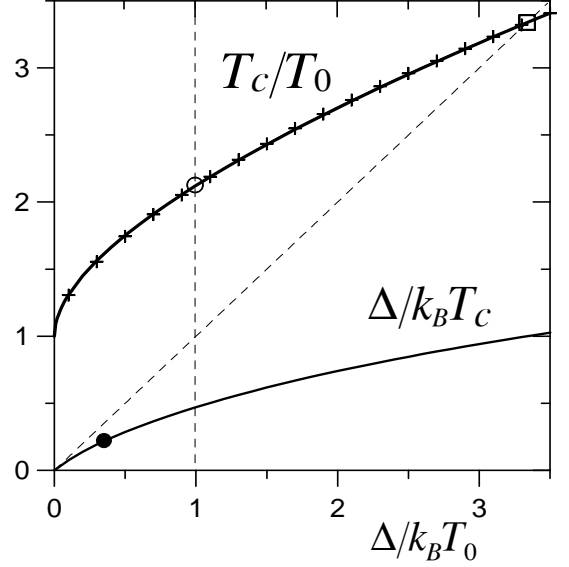


FIG. 2: T_c/T_0 and $\Delta/k_B T_c$ as functions of the gap in units of $k_B T_0$. Crosses are the approximation (9) for small $\Delta/k_B T_0$. Dot, circle and square mean $\Delta/k_B T_c = 0.22$, $\Delta = k_B T_0$ and $\Delta = k_B T_c$, respectively.

$(9/2)(1-z)^{3/2}$ for $z \in [0.8, 1]$ and $g_{3/2}(z) \simeq \exp[z] - 1$ for $z \in [0.0, 0.8]$, and that for $\Delta > 0$, $T_c/T_0 > 1$ and $z_{1c} = \exp[-\Delta/k_B T_c] = \exp[-(\Delta/k_B T_0)T_0/T_c]$ then $g_{3/2}(z_{1c})$ can be approximated by

$$\begin{cases} \zeta(3/2)/(1 + (3/2)(1 - z_{1c})^{1/2} + (9/2)(1 - z_{1c})^{3/2}) \\ \quad \text{if } \Delta/k_B T_0 \in [0, 0.22 T_c/T_0] \\ \exp[z_{1c}] - 1 \quad \text{if } \Delta/k_B T_0 \in [0.22 T_c/T_0, \infty] \end{cases} \quad (6)$$

Then, for small values of $\Delta/k_B T_0 < 0.22 T_c/T_0$ or $\Delta/k_B T_c < 0.22$, the critical temperature takes the following form

$$T_c \simeq \left[1 + 3/2 (1 - z_{1c})^{1/2} + 9/2 (1 - z_{1c})^{3/2} \right]^{2/3} T_0 \quad (7)$$

which it can be approximated after expansion around $\Delta/k_B T_c = 0$ by

$$\frac{T_c}{T_0} \simeq 1 + (\Delta/k_B T_c)^{1/2} - (\Delta/k_B T_c)/4 + \frac{35}{12}(\Delta/k_B T_c)^{3/2} + \dots \quad (8)$$

We use the structure of the last expansion to propose

$$\frac{T_c}{T_0} \simeq 1 + (\Delta/k_B T_c)^{1/2} - A(\Delta/k_B T_c) + B(\Delta/k_B T_c)^{3/2} \quad (9)$$

with $A = 0.0277$ and $B = 1.3099$ such that the last expression reproduces the values at the open circle and square of Fig. 2. In this Fig. 2 crosses represent expression (9). In the same figure we plot $\Delta/k_B T_c$ as a function of $\Delta/k_B T_0$, where the dot means $\Delta/k_B T_c = 0.22$.

For values of $\Delta/k_B T_0 > 0.22 T_c/T_0$ or $\Delta/k_B T_c > 0.22$ the critical temperature can be approximated using $g_{3/2}(z_{1c}) \simeq \exp[\exp[-\beta_c \Delta]] - 1$, then

$$T_c \simeq \left(\frac{\zeta(3/2)}{\exp[\exp[-\beta_c \Delta]] - 1} \right)^{2/3} T_0 \quad (10)$$

and

$$\Delta/k_B T_0 \simeq -(T_c/T_0) \ln(\ln[1 + \zeta(3/2)/(T_c/T_0)^{3/2}]). \quad (11)$$

Special values of the critical temperature are those for $\Delta/k_B T_c = T_0/T_c$ and $\Delta/k_B T_c = 1$. These values are $T_c/T_0 = 2.1228$ and 3.3376 , which are shown in Fig. 2 as open circle and square, respectively.

B. Condensed fraction

For $T < T_c$ the number of particles N_0 in the energy ground state is a “large” fraction of the total number N of particles in the system. The condensed fraction is $N_0/N = (N - N_e)/N = 1 - N_e/N$, where using the ratio between (2) and (4) we arrived to

$$N_0/N = 1 - \beta_c^{3/2} g_{3/2}(z_0)/[\beta^{3/2} g_{3/2}(z_{0c})], \quad (12)$$

or

$$N_0/N = 1 - \frac{T^{3/2}}{T_c^{3/2}} \frac{g_{3/2}(z_0)}{g_{3/2}(z_{0c})} \xrightarrow{\Delta \rightarrow 0} 1 - (T/T_0)^{3/2}, \quad (13)$$

with $z_0 \equiv \exp[-\beta \Delta] = z_1$ for $T < T_c$, and at $T = T_c$ $z_{0c} = z_{1c}$.

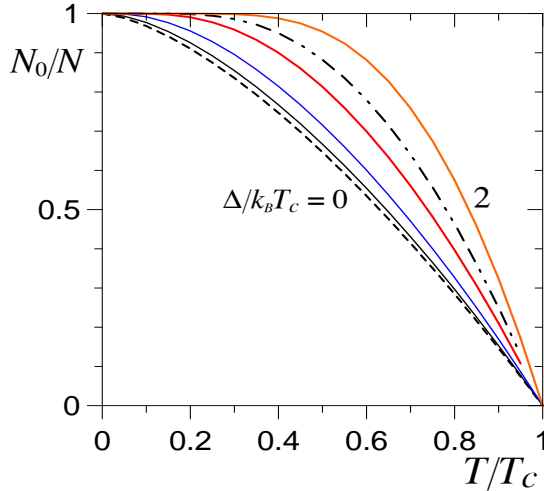


FIG. 3: Condensed fraction N/N_0 for several gap values in units of $k_B T_c$, between 0 and 2.

When $\Delta = 0$ we recover the condensed fraction for a IBG, whereas when the gap increases a higher temperature is required to diminish the condensed fraction from one. In other words, the particles in the energy ground state require a larger energy to reach the next energy level. See Fig. 3.

III. THERMODYNAMIC PROPERTIES

A. Internal energy

The internal energy $U(L^d, T)$ for bosons with energies ε_k , is

$$U(L^d, T) = \sum_{\mathbf{k}} \varepsilon_k n_k \equiv \sum_{\mathbf{k}} \frac{\varepsilon_k}{e^{\beta(\varepsilon_k - \mu)} - 1}, \quad (14)$$

Substituting (1) in the last equation, in the thermodynamic limit we obtain

$$U(L^d, T) = \varepsilon_0 N_0 + \frac{L^3 4\pi}{(2\pi)^3} \int_{0+}^{\infty} \frac{(\varepsilon_0 + \Delta + \hbar^2 k^2/2m) k^2 dk}{e^{\beta[\varepsilon_0 + \Delta + \hbar^2 k^2/2m - \mu(T)]} - 1},$$

Doing $\xi \equiv \beta[\hbar^2 k^2/2m]$, $d\xi = (\beta \hbar^2/2m) 2k dk$ and $\xi^{3/2} = (\beta \hbar^2/2m)^{3/2} k^3$, last equation becomes

$$U(L^d, T) = \varepsilon_0 N + \frac{L^3}{4\pi^2} \frac{\Delta}{\beta^{3/2}} (2m/\hbar^2)^{3/2} \int_{0+}^{\infty} \frac{\xi^{1/2} d\xi}{z_1^{-1} e^{\xi} - 1} + \frac{L^3}{4\pi^2} \frac{(2m/\hbar^2)^{3/2}}{\beta^{5/2}} \int_{0+}^{\infty} \frac{\xi^{3/2} d\xi}{z_1^{-1} e^{\xi} - 1}, \quad (15)$$

or

$$U(L^d, T)/N = \varepsilon_0 + \Delta(1 - N_0/N) + \frac{L^3}{4\pi^2} \frac{(2m/\hbar^2)^{3/2}}{\beta^{5/2} N} \Gamma(5/2) g_{5/2}(z_1), \quad (16)$$

Dividing both sides of the last equation by $k_B T$ and using Eq. (4) for N in the last term of the second member, we have

$$\frac{U(L^d, T)}{N k_B T} = \frac{\varepsilon_0}{k_B T} + \frac{\Delta(1 - N_0/N)}{k_B T} + \frac{\Gamma(5/2) g_{5/2}(z_1)}{\Gamma(3/2) g_{3/2}(z_{1c})} \left(\frac{T}{T_c} \right)^{3/2}, \quad (17)$$

where we can see that the internal energy has a first term which is the a reference energy. If we use the relation between the grand potential Ω and PV we are able to arrive to the equation of state

$$PV = (2/3)U - (2/3)N[\varepsilon_0 + (1 - N_0/N)\Delta]$$

which reduces to the well known case when Δ and ε_0 are zero.

B. Specific heat

The specific heat expression is obtained from the temperature derivative of the internal energy

$$C_V/N = d(U/N)/dT = \Delta d(1 - N_0/N)/dT + \frac{\Gamma(5/2) \beta_c^{3/2}}{\Gamma(3/2) g_{3/2}(z_{0c}) \beta^{3/2}} (5/2) k_B g_{5/2}(z_1) + \frac{\Gamma(5/2) \beta_c^{3/2}}{\Gamma(3/2) g_{3/2}(z_{0c}) \beta^{5/2}} g_{3/2}(z_1) \times [-k_B \beta^2 (\mu - \varepsilon_0 - \Delta) + \beta d\mu/dT], \quad (18)$$

where we have used

$$d/dT(\beta[\mu - \varepsilon_0 - \Delta]) = -k_B\beta^2[\mu - \varepsilon_0 - \Delta] + \beta d\mu/dT.$$

and that the temperature derivative of μ , is

$$(3/2)k_B\beta^{-1/2}g_{3/2}(z_1) + \beta^{-3/2}g_{1/2}(z_1) \times [-k_B\beta^2(\mu - \varepsilon_0 - \Delta) + \beta(d\mu/dT)].$$

For $T \leq T_c$, $\mu = \varepsilon_0$ and $d\mu/dT = 0$, then

$$C_V^-/Nk_B = \frac{(3/2)g_{3/2}(z_0)(T/T_c)^{1/2}(\Delta/k_BT_c)}{g_{3/2}(z_{0c})} + \frac{g_{1/2}(z_0)(\Delta/k_BT_c)^2}{g_{3/2}(z_{0c})(T/T_c)^{1/2}} + \frac{(5/2)\Gamma(5/2)g_{5/2}(z_0)(T/T_c)^{3/2}}{\Gamma(3/2)g_{3/2}(z_{0c})} + \frac{\Gamma(5/2)g_{3/2}(z_0)(T/T_c)^{1/2}(\Delta/k_BT_c)}{\Gamma(3/2)g_{3/2}(z_{0c})} \quad (19)$$

For $T \geq T_c$, $N_0 \simeq 0$ and

$$C_V^+/Nk_B = \frac{(5/2)\Gamma(5/2)g_{5/2}(z_1)(T/T_c)^{3/2}}{\Gamma(3/2)g_{3/2}(z_{0c})} - \frac{(3/2)\Gamma(5/2)g_{3/2}^2(z_1)(T/T_c)^{3/2}}{\Gamma(3/2)g_{3/2}(z_{0c})g_{1/2}(z_1)}$$

or

$$C_V^+/Nk_B = \frac{3(T/T_c)^{3/2}}{2g_{3/2}(z_{0c})} \left[\frac{5}{2}g_{5/2}(z_1) - \frac{3}{2} \frac{g_{3/2}^2(z_1)}{g_{1/2}(z_1)} \right] \quad (20)$$

Note that for all temperature regimes, the specific heat is ε_0 independent. However it is Δ dependent for temperatures below T_c only. For $T \rightarrow 0$ and $\Delta \neq 0$, $z_0 \rightarrow 0$ and we can approximate $g_\sigma(z_0) \simeq z_0$ by $\sigma = 5/2, 3/2$ or $1/2$. Then

$$C_V^-/Nk_B \simeq \exp(-\Delta/k_BT) \left\{ \frac{(3/2)(T/T_c)^{1/2}(\Delta/k_BT_c)}{g_{3/2}(z_{0c})} + \frac{(\Delta/k_BT_c)^2}{g_{3/2}(z_{0c})(T/T_c)^{1/2}} + \frac{(5/2)\Gamma(5/2)(T/T_c)^{3/2}}{\Gamma(3/2)g_{3/2}(z_{0c})} + \frac{\Gamma(5/2)(T/T_c)^{1/2}(\Delta/k_BT_c)}{\Gamma(3/2)g_{3/2}(z_{0c})} \right\}, \quad (21)$$

or

$$C_V^-/Nk_B \simeq \frac{\exp(-\Delta/k_BT)(T/T_c)^{3/2}}{g_{3/2}(z_{0c})} \left\{ \frac{15}{4} + 3(\Delta/k_BT) + (\Delta/k_BT)^2 \right\} \quad (22)$$

i.e., for very low temperatures the temperature dependence of the specific heat is exponential.

However, when $\Delta \rightarrow 0$ we recover the well known behavior of C_V for an ideal Bose gas at low temperatures, i.e. it is proportional to $T^{2/3}$.

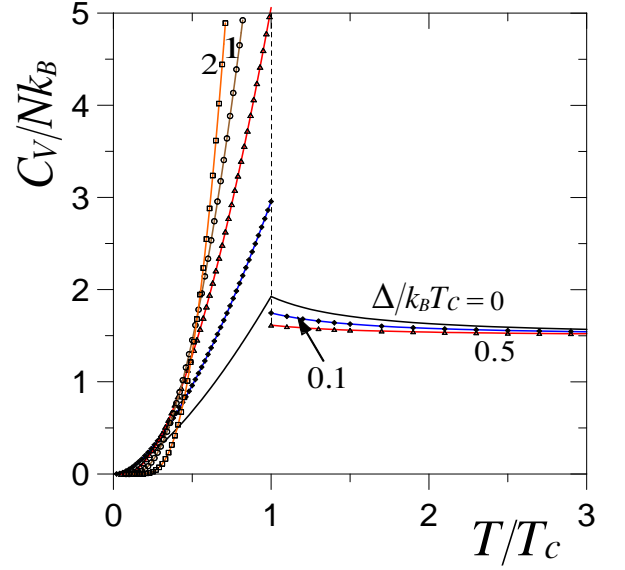


FIG. 4: Specific heat as a function of T/T_c for $\Delta/k_BT_c = 0, 0.1, 0.5, 1$ and 2 . For $\Delta/k_BT_c = 1$ and 2 , the $T/T_c > 1$ branches are not shown.

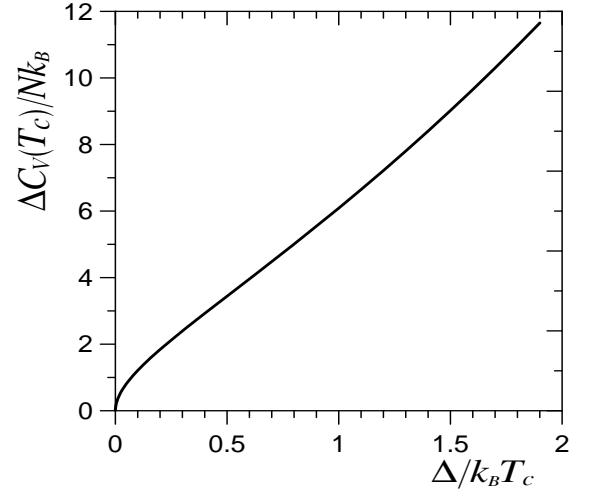


FIG. 5: Specific heat jump.

C. Jump magnitude in the specific heat

For $T = T_c$, $\mu = \varepsilon_0$ y $z_1 \rightarrow z_{0c}$

$$(C_V^- - C_V^+)/Nk_B|_{T_c} = 3(\Delta/k_BT_c) + \frac{g_{1/2}(z_{0c})(\Delta/k_BT_c)^2}{g_{3/2}(z_{0c})} + \frac{9}{4} \frac{g_{3/2}(z_{0c})}{g_{1/2}(z_{0c})}$$

In Fig. 5 we can see the specific heat jump which it is an increasing function of Δ/k_BT_c . For small Δ the specific heat jump can be approximate by $(C_V^- - C_V^+)/Nk_B|_{T_c} \simeq (10/3)(\Delta/k_BT_c)^{1/2}$.

IV. CONCLUSIONS

After calculating the BEC critical temperature, the condensed fraction, the internal energy, the isochoric specific heat and its jump magnitude at T_c , for an interactionless Bose gas whose particle energies have a gap between the ground energy and the first excited energy level, we conclude the following:

- All the calculated thermodynamic properties are independent of the magnitude of the ground state energy ε_0 , except the internal energy which is measured from the reference energy of magnitude $N\varepsilon_0$, instead of the zero ground state energy of a ideal Bose gas.

- The gap notoriously increases the magnitude of the critical temperature and brings on the appearance of a jump in the specific heat.
- Below the critical temperature and near to zero absolute, the temperature dependence of the specific heat is exponential with an exponent proportional to the gap, however when the gap becomes zero the temperature dependence of the specific heat becomes that of the IBG.

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- [1] P. Kapitza, *Nature* **141**, 74 (1938).
 - [2] J.F. Allen and A.D. Misener, *Nature* **141**, 75 (1938).
 - [3] F. London, *Nature* **141**, 643 (1938).
 - [4] A. Einstein, Quantentheorie des einatomigen idealen gas, Sitzungsberichte der Preussischen Akademie der Wissenschaften 261-267 (1924); A. Einstein, Quantentheorie des einatomigen idealen gas 2, Sitzungsberichte der Preussischen Akademie der Wissenschaften 3-14 (1925).
 - [5] W.H. Keesom and H.P. Keesom, *Physica* **2**, 557 (1935).
 - [6] F. London, *Superfluids* Vol. II (John Wiley & Sons, New York, 1954)p. 53.
 - [7] M. Toda, *Progr. Theoret. Phys.* **6**, 458 (1951); T. Matsubara, *Progr. Theoret. Phys.* **6**, 458 (1951).
 - [8] M. Girardeau and R. Arnowitt, *Phys. Rev.* **113**, 755 (1959).
 - [9] N. M. Hugenholtz and D. Pines, *Phys. Rev.* **116**, 489 (1959).
 - [10] R. Kronig and W. G. Penney, *Proc. R. Soc. A* **130**, 499 (1931).
 - [11] I. Tamm, *Z. Phys.* **76**, 849 (1932).